

Weak-coupling Treatment of Electronic (Anti-)Ferroelectricity in the Extended Falicov-Kimball Model

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Abstract. We study the (spinless) Falicov-Kimball model extended by a finite band width (hopping t_f) of the localized (f -) electrons in infinite dimensions in the weak-coupling limit of a small local interband Coulomb correlation U for half filling. In the case of overlapping conduction- and f -bands different kinds of ordered solutions are possible, namely charge-density wave (CDW) order, electronic ferroelectricity (EFE) and electronic antiferroelectricity (EAFE). The order parameters are calculated as a function of the model parameters and of the temperature. There is a first-order phase transition from the CDW-phase to the EFE- or EAFE-phase. The total energy is calculated to determine the thermodynamically stable solution. The quantum phase diagrams are calculated.

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1 Introduction

One of the simplest lattice models for strongly correlated electron systems, the Falicov-Kimball model (FKM) [1], consists of two types of spinless electrons, namely delocalized band (c -) electrons and localized f -electrons, and a local Coulomb (Hubbard) interaction between c - and f -electron at the same site. The FKM was originally introduced as a model for metal-insulator and valence transitions [1]. It can also be interpreted as a model for crystallization (identifying the "heavy" f -particles with the nuclei, the c -particles with the electrons and for $U < 0$) [2]. Furthermore, the FKM is of interest for academic reasons, because it is the simplest non-trivial lattice model for correlated electron systems, for which certain exact results are available; for a recent review see Ref. [3].

A few years ago it has been suggested by Portengen *et al.* [4] that a novel ferroelectric state could be present in the mixed-valence regime of the FKM. Whereas a ferroelectric transition is usually connected with a structural phase transition [5], a purely electronic mechanism would lead to this kind of ferroelectricity suggested to occur for the FKM; it has, therefore, been termed "electronic ferroelectricity" (EFE) [4]. The origin of EFE is a non-vanishing excitonic expectation value $P_{cf} = \langle c^\dagger f \rangle$. In the case of a vanishing hybridization between c - and f -electron states and a vanishing electrical (optical) field driving inter-band transitions, the existence of a finite $P_{cf} \neq 0$ is a kind of symmetry breaking, and if the f - and c -states have different parity, the P_{cf} causes a finite electrical polarization without a driving electrical field, because of which it is "ferroelectricity".

On the other hand, from exact results available for the FKM [2,6,7] one knows that a charge density wave (CDW) phase ("chess board phase") exists at least for half filling and in the symmetric case, and no evidence for EFE in the FKM is obtained by these exact treatments. But the possibility of CDW ordering was not considered by Portengen *et al.* [4]. Later calculations [8,9,10,11] could not confirm the existence of EFE for the FKM. A divergence in the hybridization susceptibility obtained in Ref. [12] does not necessarily mean that the ground state has spontaneous hybridization $P_{cf} \neq 0$ [10].

More recently it has been shown by Batista *et al.* [13,14] that the FKM extended by a direct $f-f$ -hopping t_f , in fact, has the EFE phases with a spontaneous hybridization. Depending on the sign of t_f a ferro- or an antiferroelectric phase may exist. A CDW phase is also possible depending on the relative position of c - and f -band and on the value of the Coulomb (Hubbard) correlation U , and the quantum phase diagrams were obtained in Refs. [13,14]. In this paper we also study the spinless extended Falicov Kimball model (EFKM) suggested by Batista [13]. Batista *et al.* studied this model in one and two dimensions in the strong [13] and the intermediate coupling [14] limit. Here we study an infinite dimensional system in the weak coupling limit. We also obtain electronic ferroelectricity (EFE), electronic antiferroelectricity (EAFE) and CDW ordering. We calculate the dependence of the order parameters on temperature and on the model parameters and calculate the total energy. The resulting quantum phase diagram is qualitatively very similar to that obtained previously in the intermediate and strong coupling limit [13,14]. We also point out that this EFKM and the E(A)FE problem and phase is closely related to the

excitonic insulator phase discussed already about 40 years ago[15,16,17].

The paper is organized as follows. In Sect. 2 we describe the EFKM and point out its connections with other standard models of correlated electron systems and solid state theory. Section 3 describes our weak-coupling approximation. The results are presented in Section 4; the c - and f -electron spectral functions are calculated for different model parameters and order types, the (CDW, EFE, EAFE) order parameters and the total energy for these phases are calculated as a function of the model parameters and the temperature, and the complete quantum phase diagram is presented, before the paper closes in Sect. 5 with a short summary and conclusion.

2 Model

The extended Falicov-Kimball model (EFKM)[13] consists of two types of spinless electrons, here denoted as c - and f -electrons, and a local Coulomb (Hubbard) interaction U between c - and f -electron at the same site. The EFKM Hamiltonian reads:

$$H = \sum_{\mathbf{R}} \left(E_c c_{\mathbf{R}}^\dagger c_{\mathbf{R}} + E_f f_{\mathbf{R}}^\dagger f_{\mathbf{R}} + U c_{\mathbf{R}}^\dagger c_{\mathbf{R}} f_{\mathbf{R}}^\dagger f_{\mathbf{R}} - \sum_{\Delta n.n.} \left[t_c c_{\mathbf{R}+\Delta}^\dagger c_{\mathbf{R}} + t_f f_{\mathbf{R}+\Delta}^\dagger f_{\mathbf{R}} \right] \right) \quad (1)$$

$$= \sum_{\mathbf{k}} \left(\varepsilon_c(\mathbf{k}) c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + \varepsilon_f(\mathbf{k}) f_{\mathbf{k}}^\dagger f_{\mathbf{k}} \right) + U \sum_{\mathbf{R}} c_{\mathbf{R}}^\dagger c_{\mathbf{R}} f_{\mathbf{R}}^\dagger f_{\mathbf{R}} \quad (2)$$

Here \mathbf{R} denotes the sites of a Bravais lattice, Δ the nearest neighbor lattice vectors, \mathbf{k} the wave vectors from the first Brillouin zone, $E_{c/f}$ are the on-site one-particle matrix elements (and thus the band centers) of the c/f -electrons, and the usual nearest neighbor tight-binding assumption (of only nearest neighbor intersite matrix elements $t_{c/f}$) has been made. Therefore, the c - and f -electron dispersions are given by:

$$\varepsilon_c(\mathbf{k}) = E_c - \sum_{\Delta n.n.} t_c e^{i\mathbf{k}\Delta}, \quad \varepsilon_f(\mathbf{k}) = E_f - \sum_{\Delta n.n.} t_f e^{i\mathbf{k}\Delta} \quad (3)$$

Several standard models of solid state theory can be identified to be certain limiting cases of this EFKM (1,2). In the case of a vanishing f -electron dispersion, i.e. $t_f = 0$, we recover, of course, the standard spinless FKM[1,3]. In the case of equal, degenerate c - and f -bands, i.e. $E_f = E_c$ and $t_f = t_c$, one can identify the c -electrons with the spin-up and the f -electrons with the spin-down electrons and obtains the standard Hubbard model[18]. A particle-hole transformation for one kind of electrons, say the f -electrons, leads to an attractive interaction $-U$; then in the case $t_f = -t_c$, $E_c + U = -E_f$ the c -electron band and the f -hole band are again degenerate, and identifying again the c -electrons with the spin-up electrons and the f -holes with the spin-down electrons one has spin-degenerate fermions with an attractive (short ranged, i.e. \mathbf{k} -independent) s -like interaction, i.e. the BCS-model[19].

Finally, if the f -electron band is interpreted as valence band and the c -electron band as conduction band (of one spin direction), one recovers the standard two-band model studied frequently in semiconductor theory[20], in particular to describe optical excitations (excitons etc.) under the influence of the Coulomb interaction, only that here this Coulomb interaction is local (short ranged). In this situation the f -(valence) band is narrower than the c -(conduction) band, i.e. $|t_f| < |t_c|$, and the f - and c -states have usually a different parity, which in the simplest way can be modelled by a different sign of t_c and t_f (i.e. $t_c > 0, t_f < 0$). In our opinion it is just this fact that so many interesting and important models of solid state theory can be identified as limiting cases of the EFKM (1,2), which makes the EFKM very useful and interesting at least for academic reasons (model studies).

3 Approximation

We will use the following model assumptions: we measure energies relative to the origin of the c -band, i.e. we choose $E_c = 0$. Furthermore, we use a semielliptical model density of states for the unperturbed c -band, i.e. we assume

$$\rho_{c0}(E) = \frac{1}{N} \sum_{\mathbf{k}} \delta(E - \varepsilon_c(\mathbf{k})) = \frac{2}{\pi} \sqrt{1 - E^2} \quad (4)$$

for $-1 < E < 1$

thereby choosing half the unperturbed c -band width as our energy unit. This implies

$$\rho_{f0}(E) = \frac{1}{|t_f|} \rho_{c0}\left(\frac{E - E_f}{|t_f|}\right) \quad (5)$$

Then we are left with three parameters: the position E_f of the (center of the) f -band relative to the (center of the) c -band, the (dimensionless) f -electron hopping t_f (i.e. the relation of the f - to the c -band width), and the Coulomb (Hubbard or Falicov-Kimball) correlation U between one f - and one c -electron at the same lattice site.

To use the semielliptical model DOS (4) is a standard model assumption introduced already more than 40 years ago by Hubbard[18]. It becomes exact for a Bethe lattice in the limit of infinite coordination number. Compared to the Gaussian model DOS, which becomes exact for a d -dimensional (hyper)cubic lattice in the limit of infinite dimensions ($d \rightarrow \infty$)[21] or coordination number, the semielliptical model DOS has the advantage that the band width is finite and true band gaps can develop and that it has the squareroot band edge van Hove singularities characteristic for three dimensional systems.

With these additional model assumptions we now apply the generalized (unrestricted) Hartree-Fock approximation (HFA), which becomes correct in the weak-coupling limit of small U . Within HFA the many-body (interaction) part of the Hamiltonian (1,2) is decoupled according to

$$\begin{aligned} c_{\mathbf{R}}^\dagger c_{\mathbf{R}} f_{\mathbf{R}}^\dagger f_{\mathbf{R}} &= \langle c_{\mathbf{R}}^\dagger c_{\mathbf{R}} \rangle f_{\mathbf{R}}^\dagger f_{\mathbf{R}} + \langle f_{\mathbf{R}}^\dagger f_{\mathbf{R}} \rangle c_{\mathbf{R}}^\dagger c_{\mathbf{R}} \\ &\quad - \langle c_{\mathbf{R}}^\dagger f_{\mathbf{R}} \rangle f_{\mathbf{R}}^\dagger c_{\mathbf{R}} - \langle f_{\mathbf{R}}^\dagger c_{\mathbf{R}} \rangle c_{\mathbf{R}}^\dagger f_{\mathbf{R}} \end{aligned} \quad (6)$$

It is an unrestricted HFA because we also allow for a decoupling with respect to off-diagonal (excitonic) expectation values $\langle c_{\mathbf{R}}^\dagger f_{\mathbf{R}} \rangle$ and because we allow for a position- (\mathbf{R}) -dependence of the expectation values $\langle c_{\mathbf{R}}^\dagger c_{\mathbf{R}} \rangle$, $\langle f_{\mathbf{R}}^\dagger f_{\mathbf{R}} \rangle$ and $\langle c_{\mathbf{R}}^\dagger f_{\mathbf{R}} \rangle$. Within HFA the full Hamiltonian (1) is replaced by the effective one-particle Hamiltonian

$$H_{\text{eff}} = \sum_{\mathbf{R}} \left(\tilde{E}_{c\mathbf{R}} c_{\mathbf{R}}^\dagger c_{\mathbf{R}} + \tilde{E}_{f\mathbf{R}} f_{\mathbf{R}}^\dagger f_{\mathbf{R}} + \tilde{V}_{\mathbf{R}} \left(c_{\mathbf{R}}^\dagger f_{\mathbf{R}} + c.c. \right) \right) - \sum_{\mathbf{R}} \sum_{\Delta n.n.} \left(t_c c_{\mathbf{R}+\Delta}^\dagger c_{\mathbf{R}} + t_f f_{\mathbf{R}+\Delta}^\dagger f_{\mathbf{R}} \right) \quad (7)$$

where the effective one-particle parameters

$$\begin{aligned} \tilde{E}_{c\mathbf{R}} &= E_c + U \langle f_{\mathbf{R}}^\dagger f_{\mathbf{R}} \rangle \\ \tilde{E}_{f\mathbf{R}} &= E_f + U \langle c_{\mathbf{R}}^\dagger c_{\mathbf{R}} \rangle \\ \tilde{V}_{\mathbf{R}} &= -U P_{cf}^{\mathbf{R}} = -U \langle c_{\mathbf{R}}^\dagger f_{\mathbf{R}} \rangle \end{aligned} \quad (8)$$

have to be determined selfconsistently together with the chemical potential μ for a given total number of electrons per site $n = \frac{1}{N} \sum_{\mathbf{R}} (\langle f_{\mathbf{R}}^\dagger f_{\mathbf{R}} \rangle + \langle c_{\mathbf{R}}^\dagger c_{\mathbf{R}} \rangle)$. In this paper we study the half filled case, i.e. $n = 1$ electron per site. $\tilde{V}_{\mathbf{R}}$ corresponds to an effective, spontaneous hybridization between f - and c -electron states, which exists only if there is a nonvanishing spontaneous polarization

$$P_{cf}^{\mathbf{R}} = \langle c_{\mathbf{R}}^\dagger f_{\mathbf{R}} \rangle = \langle f_{\mathbf{R}}^\dagger c_{\mathbf{R}} \rangle \neq 0 \quad (9)$$

Without loss of generality we assume here that $P_{cf}^{\mathbf{R}}$ and $\tilde{V}_{\mathbf{R}}$ can be chosen to be real.

Concerning the position dependence of the effective one-particle parameters $\tilde{E}_{c\mathbf{R}}$, $\tilde{E}_{f\mathbf{R}}$, $\tilde{V}_{\mathbf{R}}$ either a homogeneous, translational invariant solution, i.e. no \mathbf{R} -dependence, is possible or an inhomogeneous solution with a periodic modulation of the expectation values

$$\begin{aligned} n_{f\mathbf{R}} &= \langle f_{\mathbf{R}}^\dagger f_{\mathbf{R}} \rangle = n_{f0} + \frac{1}{2} m_f \cos(\mathbf{Q} \cdot \mathbf{R}) \\ n_{c\mathbf{R}} &= \langle c_{\mathbf{R}}^\dagger c_{\mathbf{R}} \rangle = n_{c0} + \frac{1}{2} m_c \cos(\mathbf{Q} \cdot \mathbf{R}) \\ P_{cf}^{\mathbf{R}} &= \langle c_{\mathbf{R}}^\dagger f_{\mathbf{R}} \rangle = P_{cf0} \cos(\mathbf{Q} \cdot \mathbf{R}) \end{aligned} \quad (10)$$

will be assumed. Therefore, Hartree-Fock solutions with an additional ordered structure are possible, and the treatment allows for the investigation of effects as phase separation and resulting (structural) phase transitions within the (unrestricted) HFA. This is particularly important for investigations of the (E)FKM, as it is well known (from exact results available for two [2,6] or infinite[7] dimensions) that for half filling ($n = 1$) the chessboard phase forms the ground state (i.e. an A- and B-sublattice structure with different f - and c - electron occupations on the A- and B- sublattice). Though it is also known (in particular from numerical results for the original FKM in two dimensions[22,23]) that even more complex and interesting ordered phases may exist (e.g. striped phases[23]), we will restrict our investigation to the mentioned chessboard phase. This means that we assume a bipartite lattice which

can be decomposed into an A- and B-sublattice and allow for different expectation values (occupation numbers) on the A- and B-sublattice (as in the case of antiferromagnetism). Therefore, we restrict the \mathbf{Q} -vectors in Eq. 10 to the nesting vectors $\mathbf{Q} = \pi(1, 1, \dots)$ or $\cos(\mathbf{Q}\mathbf{R}) = \pm 1$ and have the possibility of two different values $n_{c,A/B}$, $n_{f,A/B}$, $P_{cf}^{A/B}$ for the expectation values depending on whether $\mathbf{R} \in A$ or $\in B$ sublattice. Then the $m_{c,f}$ introduced in Eq. 10 is already the charge density wave (CDW) order parameter, and a non-vanishing P_{cf} is the order parameter describing spontaneous polarization, i.e. electronic (anti-) ferroelectricity or an excitonic insulator.

4 Results

The selfconsistent solution of the HFA equations always yields a homogeneous, translational invariant solution without a spontaneous polarization. Then the f - and c -bands are simply shifted by the amount Un_c and Un_f , respectively. When the two bands are sufficiently far apart from each other, the lower one will be completely filled (i.e. $n_{c/f} = 1$) and the other one is empty (i.e. $n_{f/c} = 0$) as in the case of a conventional semiconductor two-band model. However, when the bands overlap, also other HFA solutions are obtained, namely either solutions with a CDW order parameter or solutions with a spontaneous polarization. The HFA solutions with an additional symmetry breaking and order parameter have the lower energy (compared to the homogeneous solution) and, therefore, describe the better and more reliable approximation to the true ground state.

To demonstrate the different types of HFA solutions obtained, several results for the (c - and f -electron) spectral functions are shown in Fig. 1 for $U = 0.4$ and $t_f = -0.61$ and four different values of E_f . In the fully (particle-hole) symmetric case $E_f = 0$, for which a half filled c -band and a half filled f -band centered around $U/2$ can be expected, a charge density wave (CDW) solution is obtained as the most stable HFA solution. This means that there are different occupation numbers $n_{cA} \neq n_{cB}$ and $n_{fA} \neq n_{fB}$ on the different A- and B-sublattices. But in this symmetric situation one has $n_{cA} = n_{fB}$ and vice versa, and $P_{cf}^{A/B} = 0$, i.e. no spontaneous polarization. Because of the superstructure a CDW gap opens in the spectral functions, and as the Fermi energy $E_F = U/2$ falls into this gap, an insulating solution with a CDW-gap is obtained. When the (center of the) f -band is shifted compared to the c -band center, a different type of HF solution is obtained, namely one with a non-vanishing cf -polarization or an effective hybridization, as shown for $E_f = 0.3$ in Fig. 1 b). As the effective hybridization is site-diagonal (local), a hybridization gap is formed and the chemical potential falls into this hybridization gap. Therefore, for the total filling $n = 1$ again an insulating ground state is obtained, this time one with a hybridization gap. This type of insulator is also termed "excitonic insulator"[15,16,17], and because of the spontaneous cf -polarization P_{cf} it is identical to the electronic ferroelectric phase[4,13,14] and is sometimes

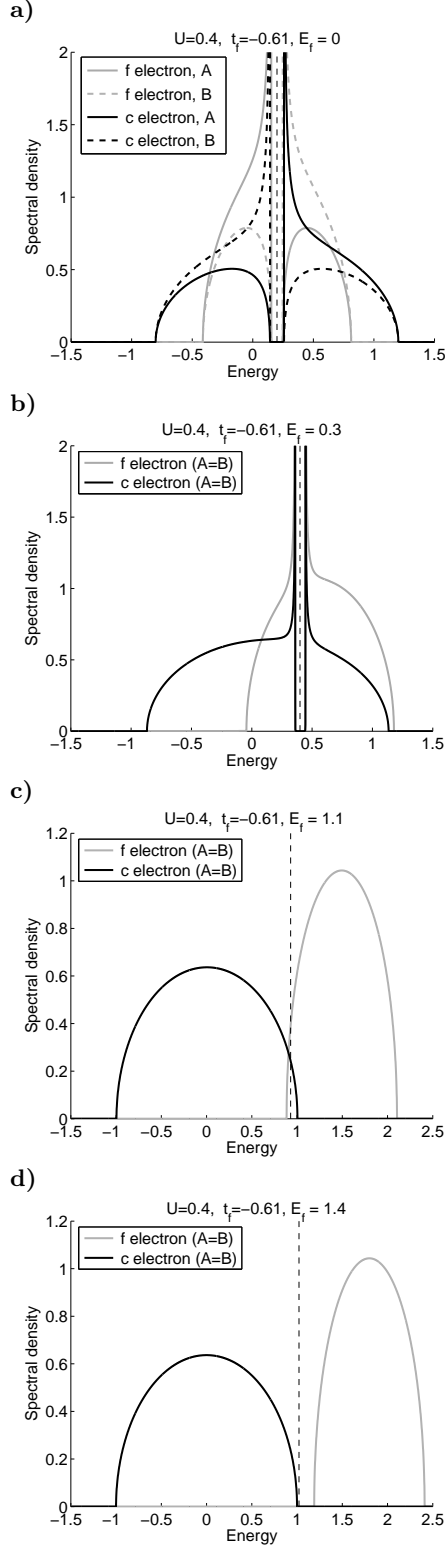


Fig. 1. c - and f -electron spectral function of the EFKM obtained within the HFA for $U = 0.4$, $t_f = -0.61$, a temperature $T = 0.002$ and different E_f

also called "excitonic Bose-Einstein condensate" (BEC) because of the non-vanishing excitonic expectation value $\langle c_{\mathbf{R}}^\dagger f_{\mathbf{R}} \rangle$. There exists another type of solution as shown in Fig.1 c), which is here obtained for $E_f = 1.1$ and corresponds to simply overlapping c - and f -bands. In this case both bands are partially filled and the ground state is, therefore, metallic. Because of the overlapping bands it is a semi-metal. In fact this homogeneous, semi-metallic phase is obtained for all values of $E_f < 1 + |t_f| - U$ as a possible HFA-solution; for low temperature T it is usually not the energetically most favorable solution, but for sufficiently high temperature $T > T_c$, where the possibly existing order parameters vanish, it always becomes the stable phase. Finally, if E_f is further shifted upwards, a situation is reached, where the two bands no longer overlap. Then the lower band is totally filled and the upper band is empty, and c - and f -band are separated by a gap, because of which one has a conventional band insulator. This situation is depicted in Fig. 1 d) for $E_f = 1.4$; it is obtained for $E_f + U - |t_f| > 1$.

The CDW phase and the "electronic ferroelectric" phase (with a spontaneous polarization) are phases with a true symmetry breaking and an order parameter. We have calculated these order parameters as a function of the different parameters U, t_f, E_f and as a function of temperature T . In Fig. 2 the CDW order parameter m_c is plotted as a function of E_f for fixed $U = 0.8$ and temperature $T = 0.002$ and three values of t_f . Obviously, within the HFA a CDW is not only obtained for the symmetric case $E_f = 0$ but in a rather large interval of E_f -values around 0. The CDW order parameter m_c remains constant up to a critical value of E_f depending on t_f , where m_c abruptly disappears. This means, as a function of E_f a first-order (quantum) phase transition is obtained for the CDW order parameter m_c . The E_f -dependence of the ferroelectric

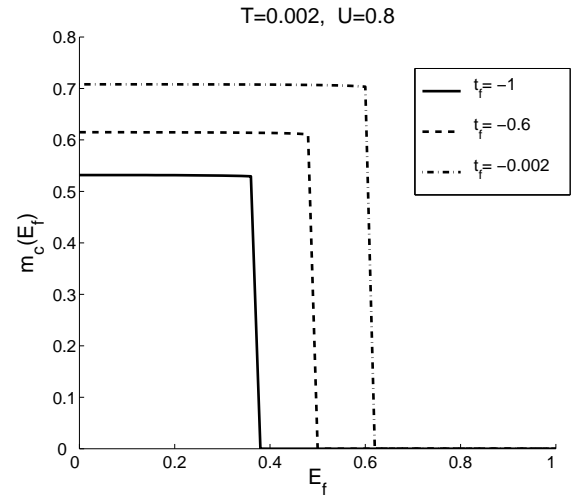


Fig. 2. CDW order parameter $m_c = |n_{cA} - n_{cB}|$ for $U = 0.8, T = 0.002$ as a function of E_f for different t_f

order parameter P_{cf} is shown in Fig.3 for fixed $t_f = -0.4$ and different U . Obviously, a HFA solution with a non-vanishing $P_{cf} \neq 0$ is obtained for all E_f smaller than a critical value $E_{fc}(U)$, which depends on the value of U . $P_{cf}(E_f)$ vanishes continuously when approaching E_{fc} , i.e. one has a quantum phase transition of second order from the ferroelectric to the homogeneous phase without symmetry breaking. Altogether all three types of HFA solu-

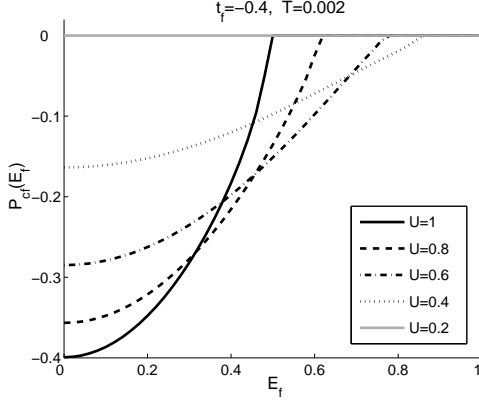


Fig. 3. Ferroelectric order parameter (spontaneous polarization) P_{cf} for $t_f = -0.4, T = 0.002$ as a function of E_f for different values of U

tions (CDW, spontaneous polarization and homogeneous without symmetry breaking) exist for the same parameters, at least for sufficiently small values of $|E_f|$. Then one has to calculate the total energy to decide which HFA-solution is the most stable one and comes closest to the true ground state. In Fig. 4 we show the dependence of the total HFA energy on E_f for the three different possible solutions for $U = 0.8, t_f = -0.31$. One observes that for $E_f = 0$ and a small interval around 0 the CDW solution is energetically the most stable one. The energy of the CDW state increases linearly with increasing $|E_f|$, while the energies of the other HFA states increase slower with increasing E_f . At some value of E_f the energy curves cross, and from that critical value E_{fc1} on the EFE solution with a spontaneous polarization is energetically the most favorable one up to a second critical E_{fc2} , where the FE solution merges into the homogeneous unpolarized HFA solution. At this value E_{fc2} the EFE order parameter vanishes (continuously, cf. Fig. 3), i.e. there is a second order quantum phase transition from the EFE to the homogeneous, unpolarized solution. A CDW-solution exists also up to E_{fc2} , but from E_{fc1} on it is no longer the most stable HFA-solution. Therefore, there is a first order quantum phase transition from the CDW solution to the EFE solution at E_{fc1} .

So far we have presented and discussed solutions for negative t_f . In the case of positive $t_f > 0$ the CDW-solutions are completely unaffected; but the EFE solution turns out to be unstable. Instead of this another phase with a symmetry breaking and order parameter exists, namely a phase with an AB-sublattice structure and dif-

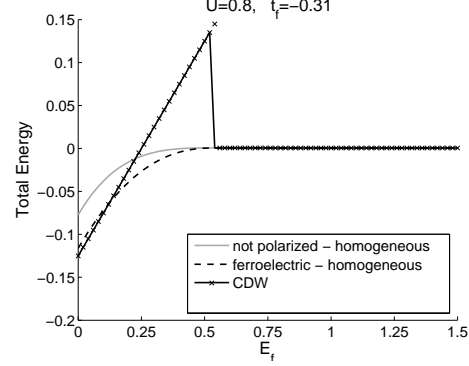


Fig. 4. Total energy of the different HFA-solutions for $U = 0.8, t_f = -0.31$ as a function of E_f

ferent (opposite but equal in magnitude) polarizations on the A- and B-sublattice, i.e. $P_{cf}^A = -P_{cf}^B \neq 0$. When the phase with a homogeneous spontaneous polarization is termed "electronic ferroelectric (EFE)" phase, the corresponding phase with non-vanishing but opposite polarizations on neighboring sites must be called "electronic anti-ferroelectric (EAFE)" phase. For $U = 0.8$ and different $t_f > 0$ the polarizations on the two sublattices are shown in Fig. 5 as a function of E_f . Obviously, except for the different sign the EAFE order parameter behaves completely analogous as the EFE order parameter in the case $t_f < 0$ (cf. Fig. 3).

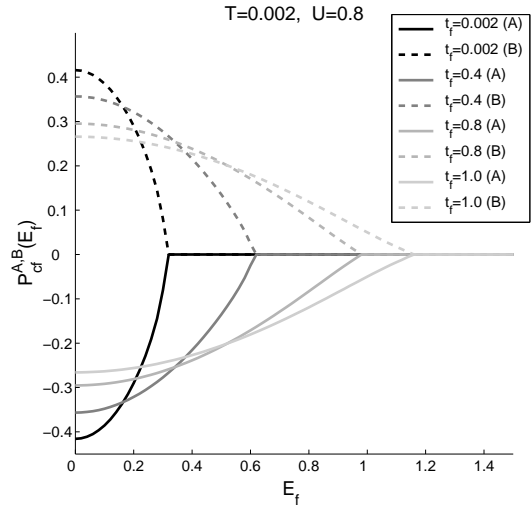


Fig. 5. Spontaneous polarization $P_{cf}^{A/B}$ on the A- and B-sublattice as a function of E_f for $U = 0.8$ and different positive $t_f > 0$

The temperature (T -) dependence of the CDW order parameter m_c is depicted in Fig. 6 for $E_f = 0, t_f = -0.4$ and different U . As it has to be expected from a HFA treatment, the order parameter behaves mean-field like and vanishes continuously (second order phase tran-

sition) at a critical temperature T_c (with a critical index of $\frac{1}{2}$); obviously T_c increases with increasing U . Also the T -dependence of the EFE order parameter P_{cf} , shown in Fig.7 for $U = 0.8, t_f = -0.4$ and different E_f is mean-field like, and P_{cf} vanishes at a T_c depending on E_f .

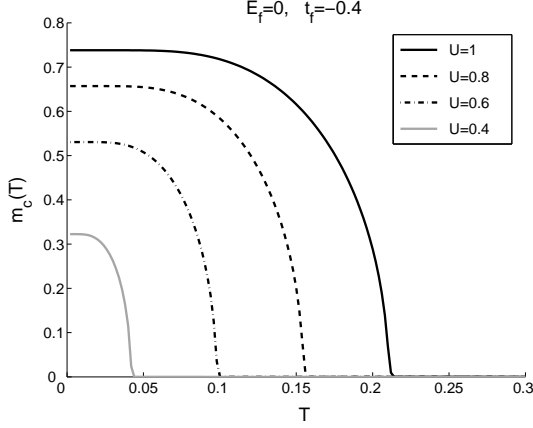


Fig. 6. Temperature dependence of the CDW order parameter m_c for $E_f = 0, t_f = -0.4$ and different U .

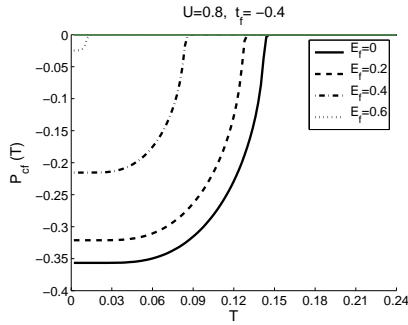


Fig. 7. Temperature dependence of the EFE order parameter P_{cf} for $U = 0.8, t_f = -0.4$ and different E_f .

The complete phase diagram obtained within the HFA is shown in Fig. 8 for fixed $U = 0.8$ in the $E_f - t_f$ -plane. We see that – besides the trivial phases of a completely filled f - or c -band (for $n = 1$) – the CDW phase and the EFE as well as the EAFE phase exist. The CDW phase becomes broadest for $t_f = 0$, i.e. for the original FKM[1]. Otherwise this line $t_f = 0$ is just the phase boundary between EAFE and EFE phase. Therefore, just for the original FKM, i.e. for $t_f = 0$, no spontaneous polarization and no (anti-)ferroelectricity has to be expected. This is in accordance with the fact that for the original FKM the f -occupation operator $f_{\mathbf{R}}^\dagger f_{\mathbf{R}}$ at each site is an exactly conserved quantity (commuting with the Hamiltonian), i.e. one has a conservation law for each lattice site \mathbf{R} . But

this special case $t_f = 0$ is an unstable fixed point: an arbitrarily small finite (positive or negative) $t_f \neq 0$ leads to an EAFE or EFE phase with a symmetry breaking and a finite order parameter. Altogether this phase diagram is in complete agreement with the one obtained previously by different methods in the case of strong[13] and intermediate[14] coupling for one- and two-dimensional systems. The same kind of phase diagram is also obtained in the weak-coupling limit, in which the HFA applied here is valid.

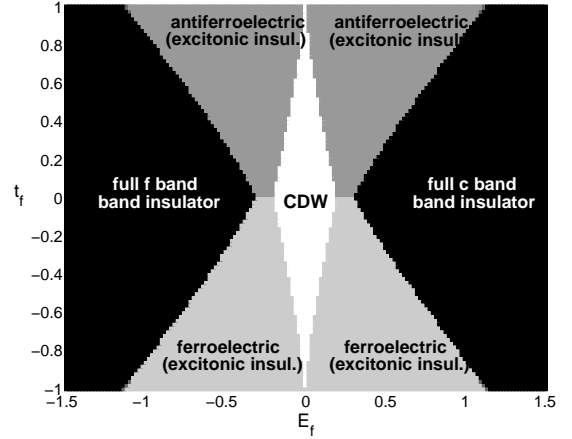


Fig. 8. EFKM phase diagram in the $E_f - t_f$ -plane for $U = 0.8$

5 Conclusion

We have investigated the extended Falicov-Kimball model (EFKM), i.e. a spinless two-band model with a finite band width (hopping) of both, the c - and the f -electrons, and a short-ranged (site diagonal, i.e. Hubbard like) Coulomb interaction U between f - and c -electrons. We have considered the weak-coupling limit of small U , in which case the (unrestricted) Hartree-Fock approximation (HFA) becomes applicable. For a total number of $n = 1$ electron per site different ground states are obtained depending on the parameters, namely either the (trivial) cases of completely filled c - or f -band, states with a non-vanishing, spontaneous $c - f$ -polarization P_{cf}^R and a CDW-state with an A-B-sublattice structure and different c - and f -electron fillings on the sites of the A- and B-sublattice as in the case of antiferromagnetism. In both cases there is a symmetry breaking, and the spontaneous polarization P_{cf} and the sublattice "magnetization" (difference of the A- and B-sublattice occupation numbers) $m_{c,f} = |n_{c,f}^A - n_{c,f}^B|$ are the order parameters. The state with a spontaneous polarization (and thus hybridization) corresponds to the excitonic insulator phase discussed already about 40 years ago[15,16,17]. A spontaneous polarization is equivalent to a non-vanishing excitonic expectation value $\langle c_{\mathbf{R}}^\dagger f_{\mathbf{R}} \rangle$, and

a ground state with an excitonic expectation value is sometimes also interpreted as an excitonic Bose-Einstein condensate [13,14]. It may be connected with a spontaneous electric dipole moment (per site); therefore, the state with a translational invariant (\mathbf{R} -independent) P_{cf} can be interpreted as "electronic ferroelectricity" (EFE) [4], which is obtained for $t_f < 0$. But for $t_f > 0$ a state with alternating (opposite) $P_{cf}^{\mathbf{R}}$ on the A- and B-sublattice is obtained, which can analogously be termed and interpreted as "electronic antiferroelectricity" (EAFE) [13,14]. We have determined the phase diagram in the $E_f - t_f$ -plane, which agrees with results obtained previously by different methods [13,14].

Our conclusions are the following:

- Previous results on the EFKM, in particular the phase diagram, obtained in the strong coupling limit by means of a mapping on an xxz-spin model [13] or in the case of intermediate U and in two dimensions by means of a constrained path Monte Carlo method [14], have been confirmed. This phase diagram can also be obtained in the weak-coupling limit of small U within a simple (unconstrained) Hartree-Fock treatment (independent of the dimension).
- The excitonic insulator state exists for this kind of two-band model for a wide range of the parameters; it is equivalent to the EFE-state (for $t_f < 0$) or the EAFE-state for $t_f > 0$. It is also equivalent to the BCS-state (if one performs a particle-hole transformation for one kind of the electrons and thus comes to a model with an attractive interband interaction).
- Around the symmetric case, i.e. for (almost) coinciding band centers of the c - and f -band, another state is energetically more stable, namely the CDW-state with different and alternating c - and f -occupation on the sites of an A- and B-sublattice. In the older work on excitonic insulators [16,15,17] and on EFE [4] it has obviously not been checked, if a more stable CDW-phase exists.
- There is a first order (quantum) phase transition from the E(A)FE state to the CDW state but a second order transition from the E(A)FE phase to the homogeneous (translationally invariant) phase (without a symmetry breaking).
- The original FKM [1] with $t_f = 0$ corresponds to the phase boundary between EFE- and EAFE phase. Therefore, neither the EFE- nor the EAFE phase is stable and only the CDW-phase (and probably more complex ordered structures or phase separation away from the symmetric case) are the ordered phases for the original FKM, in agreement with previous conclusions [8,9]. However an arbitrarily small finite $t_f \neq 0$ leads either to the EFE- (for $t_f < 0$) or to the EAFE-state (for $t_f > 0$), at least sufficiently away from the symmetric case, when the CDW-state is no longer favorable.

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Note:

After completion (but before submission) of this work, which is an extract from Claudia Schneider's thesis [24], we became aware of two very recent and related papers on the EFKM [25,26]. Ref. [25] applies the slave-boson theory to an EFKM extended additionally by a one-particle hybridization term. In Ref. [26] also the HFA has been applied (to the EFKM without hybridization and two- and three-dimensional tight-binding bands), and the results are in complete agreement with our results (obtained for the semicircular model density of states, i.e. for a Bethe lattice in the limit of infinite coordination number).

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